

# Self-Avoiding Walks with Writhe

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## Abstract

We map self-avoiding random walks with a chemical potential for writhe to the three-dimensional complex  $O(N)$  Chern-Simons theory as  $N \rightarrow 0$ . We argue that at the Wilson-Fisher fixed point which characterizes normal self-avoiding walks (with radius of gyration exponent  $\nu \approx 0.588$ ) a small chemical potential for writhe is irrelevant and the Chern-Simons field does not modify the monomer-monomer correlation function. For a large chemical potential the polymer collapses.

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# 1 Introduction and Summary

Aside from their mathematical interest, self-avoiding random walks are good models for polymers which are much longer than their persistence length. In this paper, we study how these self-avoiding random walk models can be adapted to study the effects of a topological constraint on the polymer. Recent progress in experimental technique has, for the first time, allowed the direct, real-space observation of polymer conformations [1]. These studies, as well as experiments in which polymers have been subjected to torsional constraints [2], have focussed primarily on long biopolymers. While self-avoidance is important in long biomolecules such as actin or DNA, these molecules, in addition, have a *twist* rigidity. If the twist were decoupled from the conformational changes of the polymer then twist rigidity would be unimportant. However, for a closed polymer, such as a plasmid DNA loop, there is a topological invariant, namely the linking number of the two DNA backbones. Fuller's [3] now ubiquitous [4, 5, 6, 7] relation  $Lk = Tw + Wr$  provides a connection between the topological linking number  $Lk$ , the total amount of twist in the polymer  $Tw$  and the writhe of the curve  $Wr$ —a scalar which captures some geometrical information about the conformational deformations of the loop. The way that topological constraints can affect the conformational statistics of polymers is now accessible to experimental investigation. Studies of DNA force-extension curves with constrained  $Lk$  have discovered a coupling between an excess in linking number and the backbone configuration [2]. The question arises: could there be a new universality class describing the scaling regime of topologically constrained polymers?

There is currently a wealth of information on the statistics of self-avoiding random walks. In particular, a most remarkable mapping by de Gennes [8] between the critical behavior of the scalar  $O(N)$  model as  $N \rightarrow 0$  and the behavior of self-avoiding walks has allowed, via any number of schemes, a method of calculating the radius of gyration exponent  $\nu$  which measures how the radius of gyration scales with the polymer length:  $R_G \sim L^\nu$ . It is interesting then to consider the effect of the topological constraint on the radius of gyration of the closed polymer loop. The topological constraint can be added to the standard analysis via a gauge field, as noted by Brereton and Shah [9].

As we will argue, polymers with a small chemical potential for  $Lk$  fall into the same universality class as the usual self-avoiding random walk. The experimentally observed coupling arises from the non-universal details of the polymer and not from any general long-wavelength properties. A chemical potential for  $Lk$  only becomes noticeable when it exceeds a certain threshold, at which point the chain collapses [4].

So far we have focussed our attention on a chemical potential for  $Lk$ . In what follows, we turn our attention to the writhe of a curve. The introduction of a Chern-Simons

gauge field allows us to naturally and easily incorporate a chemical potential for writhe [10]. In section 2 we will show that a chemical potential for writhe is equivalent to a chemical potential for link. What is more, our model will only have one backbone to keep track of.

In section 3 we map the statistics of self-avoiding walks with a chemical potential for their writhe onto the  $N \rightarrow 0$  complex scalar Chern-Simons theory. We then argue in section 4 that at the self-avoiding fixed point controlled by  $\nu \approx 0.588$  [11] the effect of writhe is irrelevant for a small chemical potential. From this we conclude that there is no coupling between the conformations of a polymer and its writhe in the scaling regime. Finally, in section 5 we calculate moments of the writhe and find that the field-theoretic analysis disagrees with some rigorous results [12, 13]. We understand this to be a consequence of the writhe “hiding” from the long wavelength field theory in persistence length size, plectonemic regions separated from each other.

## 2 Integrating Out the Twist

The theory we develop in section 3 incorporates a chemical potential for the writhe of a closed polymer loop. While it would be difficult, experimentally, to add such a chemical potential, a chemical potential for linking number could easily be arranged. For example, DNA plasmids in the presence of topoisomerase and ATP will tend to have some non-zero excess linking number due to the bias of the added enzyme. We show in this section that a chemical potential for writhe is equivalent to a chemical potential for the linking number.

For simplicity we assume that the long-wavelength behavior of the polymer is adequately described by a simple continuum model. The free energy for this model is determined by a bending stiffness  $\kappa$  and a twist rigidity  $C$ [4]:

$$F[\mathbf{R}, \Omega] = \frac{1}{2} \int ds \left\{ \kappa \left( \frac{d^2 \mathbf{R}}{ds^2} \right)^2 + C \Omega^2 \right\}, \quad (2.1)$$

where  $\mathbf{R}(s)$  describes the conformation of the chain backbone,  $\Omega(s)$  is the twist degree of freedom and  $s$  is the curves arclength. The partition function for this model with a chemical potential  $g^2$  for the linking number is then given by

$$Z = \int [d\mathbf{R}][d\Omega] \exp \left\{ -F[\mathbf{R}, \Omega] - g^2 \left( \text{Wr}[\mathbf{R}] + \frac{1}{2\pi} \int \Omega ds \right) \right\}, \quad (2.2)$$

where the energy is measured in units of  $k_B T$ . We have used Fuller’s formula  $Lk = \text{Tw} + \text{Wr}$  explicitly to divide the linking number into the integral of the twist density  $\Omega$

and the writhe, where the writhe of the curve is

$$Wr[\mathbf{R}] = \frac{1}{4\pi} \int ds \int ds' \left( \frac{d\mathbf{R}(s)}{ds} \times \frac{d\mathbf{R}(s')}{ds'} \right) \cdot \frac{[\mathbf{R}(s) - \mathbf{R}(s')]}{|\mathbf{R}(s) - \mathbf{R}(s')|^3}. \quad (2.3)$$

The twist degree of freedom can be integrated out to yield a new effective partition function with a chemical potential for writhe:

$$Z_{\text{eff}} = \int [d\mathbf{R}] \exp \left\{ -\frac{\kappa}{2} \int \left( \frac{d^2\mathbf{R}}{ds^2} \right)^2 ds - g^2 Wr[\mathbf{R}] \right\}. \quad (2.4)$$

Unlike the twist, the writhe is non-local and can not be integrated out so easily.

In other models it may be somewhat more cumbersome to integrate out the twist degree of freedom. As an example we can consider a ribbon-like model. Once again we will parameterize the backbone by  $\mathbf{R}(s)$ , but we will use a unit vector  $\mathbf{u}(s)$  to keep track of the twist. We take this vector to be perpendicular to the backbone tangent, for instance, in DNA  $\mathbf{u}$  could point from the central backbone to one of the two sugar-phosphate strands. In terms of this parameterization, the twist density is

$$\Omega = \frac{d\mathbf{R}}{ds} \cdot \left( \frac{d\mathbf{u}}{ds} \times \mathbf{u} \right). \quad (2.5)$$

The partition function for this modified model is

$$\begin{aligned} Z = & \int [d\mathbf{R}] [d\Omega] [d\mathbf{u}] \exp \left\{ -F[\mathbf{R}, \Omega] - g^2 \left( Wr[\mathbf{R}] + \frac{1}{2\pi} \int \Omega ds \right) \right\} \\ & \times \delta \left[ \Omega - \frac{d\mathbf{R}}{ds} \cdot \left( \frac{d\mathbf{u}}{ds} \times \mathbf{u} \right) \right] \delta[\mathbf{u}^2 - 1] \delta \left[ \mathbf{u} \cdot \frac{d\mathbf{R}}{ds} \right]. \end{aligned} \quad (2.6)$$

Upon integrating out  $\mathbf{u}$ ,

$$\begin{aligned} Z = & \int [d\mathbf{R}] [d\Omega] \det^{-1} \left[ \frac{\delta \left[ \Omega - \frac{d\mathbf{R}}{ds} \cdot \left( \frac{d\mathbf{u}}{ds} \times \mathbf{u} \right), \mathbf{u}^2 - 1, \mathbf{u} \cdot \frac{d\mathbf{R}}{ds} \right]}{\delta \mathbf{u}} \right] \\ & \times \exp \left\{ -F[\mathbf{R}, \Omega] - g^2 \left( Wr[\mathbf{R}] + \frac{1}{2\pi} \int ds \Omega \right) \right\}. \end{aligned} \quad (2.7)$$

The determinant is an isotropic functional of the backbone tangent. This functional can be expanded in powers of  $d\mathbf{R}/ds$ . Since at distances large compared to the persistence length any local isotropic model flows to the random walk fixed point we will, again, only consider the effective partition function given in (2.4).

### 3 Mapping to $N \rightarrow 0$ Scalar Chern-Simons Theory

In this section, we map the  $N \rightarrow 0$ ,  $O(N)$  complex scalar field theory with a Chern-Simons gauge field to a self-avoiding random walk with a chemical potential for writhe. The Chern-Simons term is introduced because after functionally-integrating it out we obtain an expression for the writhe of the self-avoiding random walk described by the scalar theory [9, 10]. A similar procedure to this one was used to study the area of walks in two-dimensions by Cardy [14] and the linking number of a pair of walks where one walk fills space [9], though in both those cases the gauge field had the standard Maxwell potential  $F_{\mu\nu}^2$ .

We start by considering the Wilson loop along a closed path  $\Gamma$  for a Chern-Simons gauge theory with coupling  $g$ . Namely

$$\begin{aligned} C[\Gamma] &\equiv \left\langle \exp \left\{ i \oint_{\Gamma} dR_{\mu} A^{\mu} \right\} \right\rangle \\ &= \int [d\mathbf{A}] \exp \left\{ i \int ds \frac{dR_{\mu}}{ds} \cdot A^{\mu}(\mathbf{R}(s)) \right\} \exp \left\{ -\frac{1}{4g^2} \int d^3x \mathbf{A} \cdot \nabla \times \mathbf{A} \right\} \exp \{-S_{\text{gf}}\}, \end{aligned} \quad (3.1)$$

where we have added the gauge fixing term,

$$S_{\text{gf}} = \frac{1}{2\Delta} \int d^3x (\nabla \cdot \mathbf{A})^2. \quad (3.2)$$

Though the Wilson loop is gauge-invariant, in practice we must select a gauge to compute it. We choose the Landau gauge ( $\Delta \rightarrow 0$ ) so that the Chern-Simons propagator takes on a simple form:

$$\langle A_i(q) A_k(-q) \rangle = 2g^2 \frac{i\epsilon_{ijk} q_j}{q^2} + \Delta \frac{q_i q_k}{q^4} \xrightarrow{\Delta \rightarrow 0} 2g^2 \frac{i\epsilon_{ijk} q_j}{q^2}. \quad (3.3)$$

As we shall show, the antisymmetry of the propagator in this gauge simplifies the renormalization group analysis by eliminating a number of Feynman graphs.

Writing

$$A^{\mu}(\mathbf{R}(s)) = \int d^3x \delta^3[\mathbf{x} - \mathbf{R}(s)] A^{\mu}(\mathbf{x}) \quad (3.4)$$

we can perform the functional integration in (3.1) to find

$$\left\langle \exp \left\{ i \oint_{\Gamma} dR_{\mu} A^{\mu} \right\} \right\rangle = \exp \left\{ -g^2 \text{Wr}[\Gamma] \right\}. \quad (3.5)$$

The writhe of any closed path is therefore determined by the line integral of the Chern-Simons gauge field.

To include self-avoidance, we employ a generalization of de Gennes' mapping of self-avoiding random walks onto the  $N \rightarrow 0$ ,  $O(N)$  real scalar field theory [8]. It is useful

instead to consider the  $N \rightarrow 0$ ,  $O(N)$  complex scalar field theory which is equivalent[15]. Recall that the mapping proceeds by considering the high temperature series for the  $N$  component complex Ising model with Hamiltonian

$$H = \sum_{\langle i,j \rangle} \mathbf{s}_i^\dagger \cdot \mathbf{s}_j + \text{c.c} \quad (3.6)$$

where  $\langle i, j \rangle$  denotes nearest neighbors and  $\mathbf{s}_j$  is an  $N$ -component complex vector field with  $\mathbf{s}_i^\dagger \cdot \mathbf{s}_i = N$ . The discrete version of the Wilson line for a path from  $\mathbf{0}$  to  $\mathbf{x}$  is

$$C[\Gamma] = \left\langle \exp\left\{i \sum_{\Gamma} A_{ij}\right\} \right\rangle \quad (3.7)$$

where  $A_{ij}$  is a field defined on the link connecting sites  $i$  and  $j$  and the sum is along the path  $\Gamma$  which connects  $\mathbf{0}$  and  $\mathbf{x}$ . In order to weight each path by its writhe, we can include in the series expansion the corresponding Wilson line and integrate out  $\mathbf{A}$  to give each path a chemical potential  $g^2$  for writhe. Incorporation of this phase is straightforward—we replace the Hamiltonian in (3.6) with a modified one:

$$H = \sum_{\langle i,j \rangle} \mathbf{s}_i^\dagger \cdot \mathbf{s}_j U_{ij} + \text{c.c.}, \quad (3.8)$$

where  $U_{ij} = \exp\{iA_{ij}\}$ . We recognize this Hamiltonian as that for a lattice gauge theory [16], where the local gauge symmetry is

$$\begin{aligned} U_{ij} &\rightarrow U_{ij} e^{i(\theta_i - \theta_j)} \\ \mathbf{s}_i &\rightarrow \mathbf{s}_i e^{i\theta_i} \end{aligned} \quad (3.9)$$

where  $\theta_i$  is arbitrary. In the continuum limit the transformation of  $U_{ij}$  becomes  $\mathbf{A} \rightarrow \mathbf{A} + \partial\theta$ , the usual gauge transformation. Taking the continuum limit [16] of (3.9) and including the Chern-Simons term leads us to the  $O(N)$  complex scalar Chern-Simons action

$$S = \int d^3x \left( e \left| (\partial - i\mathbf{A}) \vec{\psi} \right|^2 - \mu |\vec{\psi}|^2 + u |\vec{\psi}|^4 + \frac{1}{4g^2} \mathbf{A} \cdot \nabla \times \mathbf{A} \right), \quad (3.10)$$

where  $\vec{\psi}$  is an  $N$ -component, complex scalar field,  $u$  is the monomer-monomer repulsion and  $\mu$  is the chemical potential to add a monomer or step. Note that, though the scalar field theory has a  $U(N)$  symmetry, we are only gauging the diagonal  $U(1)$ . There is no quantization condition on  $g$  as is typical in non-Abelian Chern-Simons theories [17] or in the presence of magnetic monopoles [18, 19], which are not part of this theory.

Recalling the mapping [8, 15], the correlation function is

$$\tilde{G}_\Gamma(\mathbf{x}) = \lim_{N \rightarrow 0} \frac{1}{N} \left\langle \vec{\psi}^\dagger(\mathbf{x}) \cdot \vec{\psi}(\mathbf{0}) \right\rangle = \sum_L \Upsilon(\mathbf{x}; L) e^{\mu L} \quad (3.11)$$

where  $\Upsilon(\mathbf{x}; L)$  is the sum over all paths of length  $L$  that connect  $\mathbf{0}$  to  $\mathbf{x}$  weighted by  $\exp\{-g^2 Wr\}$  and  $(\cdot)$  is the inner product defined on the  $N$ -component internal space. This correlation function is not gauge invariant: to make it gauge invariant we could add a Wilson line to the correlation function. The arbitrariness of the path we choose to connect  $\mathbf{0}$  to  $\mathbf{x}$  will lead to an arbitrary value of the writhe since the expression in (2.3) is manifestly not additive—it depends on the whole curve.

For a closed polymer loop, however, we can consider the correlation function

$$\begin{aligned} G_{\Gamma}^C(\mathbf{x}) &\equiv \frac{1}{N^2} \sum_{\alpha\beta} \left\langle s_{\mathbf{0}}^{\alpha} (s_{\mathbf{0}}^{\beta})^* (s_{\mathbf{x}}^{\alpha})^* s_{\mathbf{x}}^{\beta} \right\rangle \\ &\rightarrow \frac{1}{N^2} \left\langle \vec{\psi}^{\dagger}(\mathbf{x}) \cdot \vec{\psi}(\mathbf{0}) \vec{\psi}^{\dagger}(\mathbf{0}) \cdot \vec{\psi}(\mathbf{x}) \right\rangle \end{aligned} \quad (3.12)$$

where  $\alpha$  and  $\beta$  are the indices of the  $N$  component field and  $(\cdot)$  is the inner product defined on the  $N$ -component internal space. This correlation function is gauge invariant and, in the  $N \rightarrow 0$  limit may be written as

$$G^C(\mathbf{x}) = \sum_L \Upsilon^C(\mathbf{x}; L) e^{\mu L}, \quad (3.13)$$

where now  $\Upsilon^C(\mathbf{x}; L)$  is the sum over all closed loops of length  $L$  which pass through  $\mathbf{0}$  and  $\mathbf{x}$  weighted by  $\exp\{-g^2 Wr\}$ . Upon normalizing  $\Upsilon^C(\mathbf{x}; L)$  for fixed  $L$  we may find the probability of a closed, self-avoiding walk passing through  $\mathbf{0}$  and  $\mathbf{x}$  with a chemical potential  $g^2$  for its writhe. For a monomer chemical potential  $\mu$  close to its critical value  $\mu_c$ ,  $G^C(\mathbf{x}, \mu)$  will scale as  $[|\mathbf{x}|(\mu - \mu_c)^{\nu}]$ , where  $\nu$  is the usual correlation length exponent of critical phenomena. Inverting the sum in (3.11) to find  $\Upsilon_L^C(\mathbf{x})$  will lead to a scaling form for the probability

$$P^C(\mathbf{x}; L) \propto \Xi \left( \frac{|\mathbf{x}|}{L^{\nu}} \right) \quad (3.14)$$

and so the radius of gyration of the closed self-avoiding walk will still scale as  $L^{\nu}$ . In the next section we will argue that at the self-avoiding walk fixed point (*a.k.a* the Wilson-Fisher fixed point) the Chern-Simons gauge field is *irrelevant*, and thus the presence of writhe does not change the radius of gyration of a closed polymer loop for  $g \lesssim 1$ .

## 4 Renormalization Group Results

In this section we perform a renormalization group analysis of the complex  $O(N)$  spin model coupled to a Chern-Simons gauge field in the  $N \rightarrow 0$  limit. We will show that the presence of the Chern-Simons term does not change the long-distance behavior of the four point correlation function in (3.12).

Our analysis is based on a perturbation expansion around the Wilson-Fisher fixed point of the ungauged model. At this fixed point we have the following symbolic recursion relations which define the critical behavior for self-avoiding random walks:

$$\begin{aligned}\frac{de}{dl} &= e (-\eta + f_e(e, u)), \\ \frac{d\mu}{dl} &= \mu f_\mu(e, u), \\ \frac{du}{dl} &= u f_u(e, u).\end{aligned}\tag{4.1}$$

The functions  $f_x$  can be computed, for instance, by a  $d = 4 - \epsilon$  expansion [20]. The scaling relation given in (4.1) for the coefficient  $e$  defines an anomalous dimension for the scalar fields: if this coefficient is chosen not to rescale, then its exponent is absorbed into the  $\psi$  and  $\psi^\dagger$  fields. This implies that the scalar propagator no longer scales with its naïve dimension: at the Wilson-Fisher fixed point the scalar propagator is proportional to  $k^{-2+\eta}$ . This makes the infrared power counting at the Wilson-Fisher fixed point softer than that at the Gaussian fixed point where  $\langle \psi^\dagger \psi \rangle \sim k^{-2}$ . As we shall see, this difference will prove important by keeping the corrections to (4.1) from diverging in the infrared.

In what follows we will consider how the addition of the Chern-Simons gauge field modifies these recursion relations for the self-avoiding walk field theory in three dimensions.

## 4.1 Non-Renormalization of the Gauge Field

We first show that the gauge propagator is not renormalized. This may not be surprising since the gauge field can only couple to closed scalar loops. These scalar loops generate diagrams proportional to  $N$  which vanish in the  $N \rightarrow 0$  limit (fig. 1). To prove that the gauge field does not get renormalized, we introduce an auxiliary Hubbard-Stratonovich field  $\chi$  through a new term that we will add to the action in (3.10):

$$S_\chi = \frac{1}{2} \int d^3x \left( \chi + i\sqrt{2u}|\psi|^2 \right)^2.\tag{4.2}$$

Since the  $\chi$  field enters quadratically into the action, the new partition function will simply be proportional to the old one and the equations of motion for  $\psi$ ,  $\psi^\dagger$ , and  $\mathbf{A}$  will be left unchanged:

$$\begin{aligned}Z &= \int [d\mathbf{A}][d\chi] [d\vec{\psi}] [d\vec{\psi}^\dagger] \exp \left\{ - \int d^3x \left[ e \left| (\partial - i\mathbf{A}) \vec{\psi} \right|^2 - \left( \mu - i\chi\sqrt{2u} \right) |\vec{\psi}|^2 \right] \right\} \\ &\quad \times \exp \left\{ - \int d^3x \left( \frac{1}{4g^2} \mathbf{A} \cdot \nabla \times \mathbf{A} + \frac{1}{2\Delta} (\nabla \cdot \mathbf{A})^2 + \frac{\chi^2}{2} \right) \right\}.\end{aligned}\tag{4.3}$$



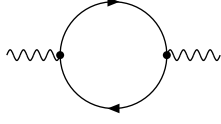


Figure 1: A correction to the gauge propagator with a closed scalar loop which vanishes in the  $N \rightarrow 0$  limit.

Since the scalar field now appears quadratically, we can integrate it out, leaving a determinant:

$$Z = \int [d\mathbf{A}][d\chi] \det^{-N} \left[ e (\partial - i\mathbf{A})^2 - (\mu - i\chi\sqrt{2u}) \right] \\ \times \exp \left\{ - \int d^3x \left( \frac{1}{4g^2} \mathbf{A} \cdot \nabla \times \mathbf{A} + \frac{1}{2\Delta} (\nabla \cdot \mathbf{A})^2 + \frac{\chi^2}{2} \right) \right\}. \quad (4.4)$$

In the  $N \rightarrow 0$  limit, the determinant does not contribute to the  $\mathbf{A} - \chi$  partition function. The Chern-Simons field  $\mathbf{A}$  is therefore a free field which keeps its naïve dimension in the renormalization process. Moreover gauge invariance implies that  $\mathbf{A}$  must scale as  $\partial$  and so, in three dimensions,  $g^2$  does not rescale:

$$\frac{dg}{dl} = 0. \quad (4.5)$$

Though the gauge coupling does not get renormalized, its presence may still renormalize the couplings  $e$ ,  $\mu$ , and  $u$ . We will explore this possibility in the next subsection.

Superficially it might appear that the same argument presented above for the  $\mathbf{A}$  field could be applied to the scalar field  $\psi$ . This would lead to the incorrect conclusion that  $\psi$  also keeps its naïve dimension upon renormalization. Of course the  $\psi$  field does get renormalized – it acquires an anomalous dimension  $\eta$  as indicated in (4.1). The argument put forward above cannot be applied to the scalar field as this field’s couplings are already  $\mathcal{O}(N)$ . The determinant that we were previously able to disregard generates just such terms, as can be seen from an expansion of  $\det^N[M] \equiv \exp(N \text{tr} \ln M)$ , where  $M$  is the operator in (4.4).

## 4.2 Perturbation Around the Wilson-Fisher Fixed Point

We start our renormalization group analysis with the recursion relations for  $e$ ,  $\mu$ , and  $u$  at the Wilson-Fisher fixed point of the ungauged  $O(N)$  complex scalar theory in the

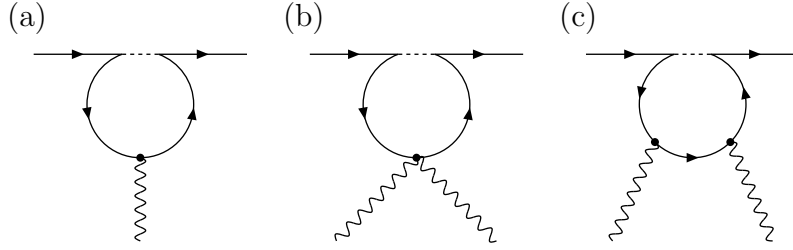


Figure 2: Corrections to the cubic and quartic gauge vertices.

$N \rightarrow 0$  limit (4.1). We will perform a one-loop perturbative expansion in the gauge field propagator.

At zeroth order in our perturbation analysis there is no gauge propagator. The lack of a dynamical gauge field severely limits the number of graphs that can modify the renormalization group equations: to one loop, there are only three of them (fig. 2). The first of these (fig. 2(a)) could contribute a correction to the single gauge field vertex:

$$\Gamma_{A\psi^\dagger\psi}^{(0)} = \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} \frac{d^d\mathbf{k}_3}{(2\pi)^d} \delta^d(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) A_i(\mathbf{k}_3) \bar{\psi}^\dagger(\mathbf{k}_2) \cdot \vec{\psi}(\mathbf{k}_1) (\mathbf{k}_1 - \mathbf{k}_2)_i. \quad (4.6)$$

The second and third graphs (figs. 2(b) and 2(c)) could modify the quartic coupling,

$$\begin{aligned} \Gamma_{AA\psi^\dagger\psi}^{(0)} = & \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} \frac{d^d\mathbf{k}_3}{(2\pi)^d} \frac{d^d\mathbf{k}_4}{(2\pi)^d} \delta^d(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3 + \mathbf{k}_4) \\ & \times A_i(\mathbf{k}_3) A_i(\mathbf{k}_4) \bar{\psi}^\dagger(\mathbf{k}_2) \cdot \vec{\psi}(\mathbf{k}_1). \end{aligned} \quad (4.7)$$

In a gauge invariant regularization scheme such as dimensional regularization, fig. 2(a) is identically zero. By gauge invariance, the other two graphs must then cancel. Therefore to one loop order, the presence of a non-dynamical gauge field does not modify the recursion relations given in (4.1) and so leaves the critical behavior of our model unchanged. This confirms that  $\mathbf{A}$  scales as  $\partial$  when  $\mathbf{A}$  is not dynamical.

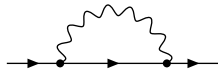


Figure 3: Wavefunction renormalization of the  $\psi$  field.

We now consider terms that are dependent on the gauge propagator. At one loop, there is just one new graph in the Landau gauge that could contribute to the scalar propagator (fig. 3):

$$\begin{aligned} \Gamma_{\psi^\dagger\psi}^{(1)} &= 2g^2 \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} \delta^d(\mathbf{k}_1 + \mathbf{k}_2) \vec{\psi}^\dagger(\mathbf{k}_2) \cdot \vec{\psi}(\mathbf{k}_1) \\ &\quad \times \int \frac{d^d\mathbf{q}}{(2\pi)^d} (2\mathbf{k}_1 - \mathbf{q})_i \frac{i\epsilon_{ijk}q_j}{q^2} (-2\mathbf{k}_2 - \mathbf{q})_k \frac{1}{|\mathbf{k}_1 - \mathbf{q}|^{2-\eta}}. \end{aligned} \quad (4.8)$$

Naïve power counting with  $\eta = 0$  would have this graph diverging logarithmically in three dimensions; however the anomalous dimension of the scalar field ( $\eta \approx 0.016$ ) makes this graph finite in the infrared. In fact,  $\Gamma_{\psi^\dagger\psi}^{(1)}$  vanishes identically because the integrand in (4.8) is a contraction of symmetric and antisymmetric tensors. We conclude that the presence of the gauge field does not modify the recursion relations for either  $e$  or  $\mu$  to one loop.

We have already seen that there are no corrections to the gauge field vertices at one loop order in the absence of the Chern-Simons potential. We now verify that these vertices remain unchanged in the presence of the dynamical propagator. Consider the one loop corrections to  $\Gamma_{A\psi^\dagger\psi}^{(0)}$ . The one loop graphs which renormalize this vertex are shown in fig. 4. As a concrete example, we consider the first of these (fig. 4(a)) which is

$$\begin{aligned} \Gamma_{A\psi^\dagger\psi}^{(1a)} &= 2g^2 \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} \frac{d^d\mathbf{k}_3}{(2\pi)^d} \delta^d(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) A_l(\mathbf{k}_3) \vec{\psi}^\dagger(\mathbf{k}_2) \cdot \vec{\psi}(\mathbf{k}_1) \\ &\quad \times \int \frac{d^d\mathbf{q}}{(2\pi)^d} (\mathbf{k}_1 + 2\mathbf{q} - \mathbf{k}_2)_l \frac{(2\mathbf{k}_1 + \mathbf{q})_i}{|\mathbf{k}_1 - \mathbf{q}|^{2-\eta}} \frac{i\epsilon_{ijk}q_j}{q^2} \frac{(-2\mathbf{k}_2 + \mathbf{q})_k}{|\mathbf{k}_2 + \mathbf{q}|^{2-\eta}}. \end{aligned} \quad (4.9)$$

The relevant part of this graph is the part proportional to  $\mathbf{k}_1 - \mathbf{k}_2$ . Terms with higher

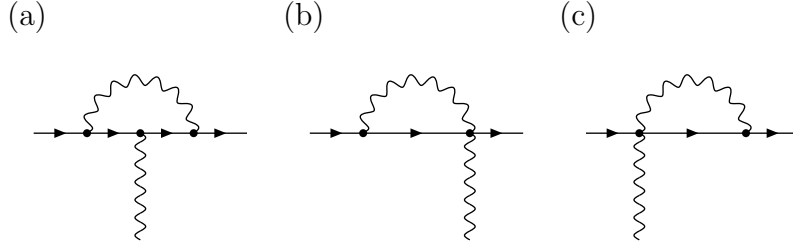


Figure 4: Corrections to the single gauge field vertex (4.6).

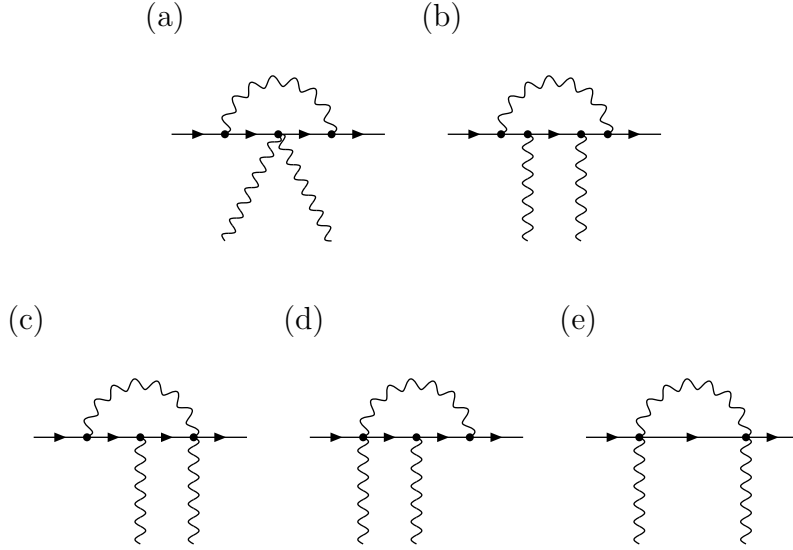


Figure 5: Corrections to the quartic gauge vertex (4.7).

powers of the external momenta generate irrelevant operators and terms with higher powers of  $q$  generate infrared-finite corrections which do not alter the scaling behavior. Leaving these uninteresting pieces behind, we now have

$$\begin{aligned} \Gamma_{A\psi^\dagger\psi}^{(1a)} &= 2g^2 \int \frac{d^d\mathbf{k}_1}{(2\pi)^d} \frac{d^d\mathbf{k}_2}{(2\pi)^d} \frac{d^d\mathbf{k}_3}{(2\pi)^d} \delta^d(\mathbf{k}_1 + \mathbf{k}_2 + \mathbf{k}_3) A_l(\mathbf{k}_3) \vec{\psi}^\dagger(\mathbf{k}_2) \cdot \vec{\psi}(\mathbf{k}_1) \\ &\times \int \frac{d^d\mathbf{q}}{(2\pi)^d} (\mathbf{k}_1 - \mathbf{k}_2)_l \frac{i\epsilon_{ijk} q_i q_j q_k}{q^{6-2\eta}}. \end{aligned} \quad (4.10)$$

Once again, a non-zero  $\eta$  saves us from having a potentially logarithmic infrared divergence for  $d = 3$ . But again, the relevant part of  $\Gamma_{A\psi^\dagger\psi}^{(1a)}$  vanishes due to the antisymmetry of the Chern-Simons propagator. By power counting, the other two graphs (figs. 4(b) and 4(b)) can be shown to generate (at worst) finite corrections. These graphs in fact vanish as they are both integrals of odd functions.

The possible corrections to the quartic gauge coupling (4.7) are depicted in fig. 5. None of these graphs will contribute to the renormalization of the vertex however: by power counting arguments they are all finite at the Wilson-Fisher fixed point. Indeed the relevant parts of all of these graphs vanish in Landau gauge due to the antisymmetric gauge propagator.

The one loop results just obtained are natural consequences of gauge invariance.

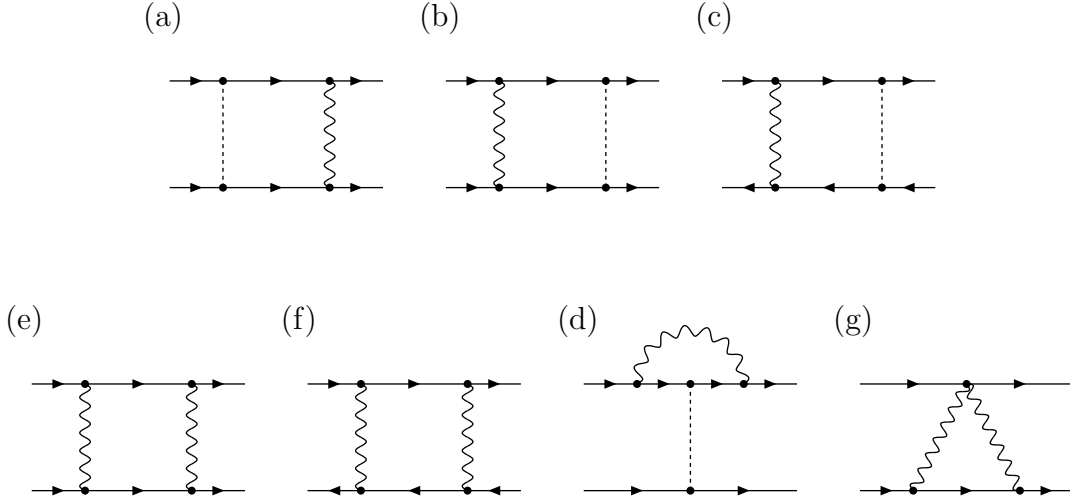


Figure 6: Vanishing corrections to the  $u$  vertex.

We must now consider the  $u$  vertex which is marginally relevant at the Wilson-Fisher fixed point. We will verify that the fixed point value for  $u$  does not lose its stability with the introduction of the gauge propagator. To see this, we consider the one loop graphs depicted in figs. 6 and 7. Once again power counting tells us that none of these graphs can generate a relevant correction to scaling (*i.e.* an infrared-divergent graph). Moreover, the relevant parts of all the graphs in fig. 6 vanish, once again due to the antisymmetry of the gauge propagator. The graph in fig. 7 on the other hand, does not vanish and generates a finite correction to  $u$ :

$$\begin{aligned}
u &= u_0 + 4g^4 \int \frac{d^d \mathbf{q}}{(2\pi)^d} \frac{\epsilon_{kji} \epsilon_{ilk} q_j q_l}{q^4} \\
&= u_0 - 4g^4 \int_0^\Lambda \frac{q^{d-1} dq}{(2\pi)^d} \frac{(d-1)f(d)}{q^2} \\
&\xrightarrow{d=3} u_0 - \frac{4g^4}{\pi^2 L_p}.
\end{aligned} \tag{4.11}$$

Here  $f(d)$  is the area of a unit  $d$ -sphere and the persistence length of the chain  $L_p$  defines the short-distance, ultraviolet cutoff  $\Lambda = L_p^{-1}$ . This term decreases the amount of self-avoidance in our random walk by a finite amount. Since a finite correction does not change the recursion relations in (4.1), this correction will not change the scaling

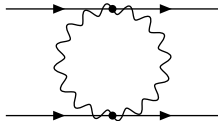


Figure 7: A finite one loop correction to the  $u$  vertex.

exponent for the radius of gyration. Nonetheless, its presence can be felt if the chemical potential for writhe  $g^2$  exceeds a certain threshold. When  $4g^4 L_p^{-1} \pi^{-2} \geq u_0$  (where  $u_0$  is the bare repulsion) the repulsive term becomes attractive and the chain collapses as it would in a bad solvent. In the case of excluded volume interactions  $u_0 \sim L_p$  (i.e.  $k_B T$  per persistence length) and the chain will collapse for  $g^4 \gtrsim (\pi/2)^2$ .

We have thus shown that the presence of a Chern-Simons field does not change the critical behavior of the  $O(N)$  complex scalar model in the  $N \rightarrow 0$  limit at one loop. Using the mappings of sections 2 and 3, we can interpret this results in terms of closed self-avoiding walks with a chemical potential for link. The presence of such a chemical potential does not affect the statistics of the random walk unless it exceeds a certain threshold, at which point the chain collapses.

## 5 Average Writhe of a Closed Loop

We have found that the presence of a small chemical potential for writhe does not change the scaling behavior of a self-avoiding random walk. Here we study the first two moments of the writhe,  $\langle Wr \rangle$  and  $\langle Wr^2 \rangle$ .

In the absence of a chemical potential  $g^2$ , a rigorous result establishes that the ensemble average of the magnitude of the writhe must scale at least as fast as the square root of the chain length [13]. Numerical results saturate this bound:  $\langle |Wr| \rangle \sim L^{\frac{1}{2}}$  [12]. We therefore expect the average of the writhe squared to scale with the length of the polymer. A simple estimate of  $\langle Wr^2 \rangle$  can be obtained by assuming that the tangents are perfectly correlated within a persistence length and completely uncorrelated at larger distances [21]. We have

$$\begin{aligned}
\langle W_I^2 \rangle &= \frac{1}{16\pi^2 Z} \int [d\mathbf{R}] e^{-F} \int ds_1 ds_2 ds_3 ds_4 \left( \frac{d\mathbf{R}(s_1)}{ds_1} \times \frac{d\mathbf{R}(s_2)}{ds_2} \right) \cdot \frac{\mathbf{R}(s_1) - \mathbf{R}(s_2)}{|\mathbf{R}(s_1) - \mathbf{R}(s_2)|^3} \\
&\quad \times \left( \frac{d\mathbf{R}(s_3)}{ds_3} \times \frac{d\mathbf{R}(s_4)}{ds_4} \right) \cdot \frac{\mathbf{R}(s_3) - \mathbf{R}(s_4)}{|\mathbf{R}(s_3) - \mathbf{R}(s_4)|^3}
\end{aligned} \tag{5.1}$$

where the free energy cost is just a bending stiffness:

$$F[\mathbf{R}] = \frac{\kappa}{2} \int ds \left( \frac{d^2 \mathbf{R}}{ds^2} \right)^2. \tag{5.2}$$

Our simplifying assumption is

$$\left\langle \frac{dR_i(s)}{ds} \frac{dR_j(s')}{ds'} \right\rangle = \begin{cases} \delta_{ij} & \text{for } |s - s'| < L_p \\ 0 & \text{otherwise} \end{cases}. \tag{5.3}$$

Using this tangent-tangent correlation function and neglecting the correlations between  $\mathbf{R}$  and  $d\mathbf{R}/ds$ , we find

$$\begin{aligned}
\langle W_I^2 \rangle &\sim \int ds_1 ds_2 ds_3 ds_4 \left\langle \frac{(\mathbf{R}(s_1) - \mathbf{R}(s_2)) \cdot (\mathbf{R}(s_3) - \mathbf{R}(s_4))}{|\mathbf{R}(s_1) - \mathbf{R}(s_2)|^3 |\mathbf{R}(s_3) - \mathbf{R}(s_4)|^3} \right\rangle \\
&\sim L_p^2 \int ds_1 ds_2 \frac{1}{|\mathbf{R}(s_1) - \mathbf{R}(s_2)|^4} \\
&\sim L_p^2 \int ds_1 ds_2 \frac{1}{L_p^2 |s_1 - s_2|^2} \\
&\sim L \left( \frac{1}{L_p} - \frac{1}{L} \right) \sim \frac{L}{L_p}.
\end{aligned} \tag{5.4}$$

Here we have used the statistics for a Gaussian chain in the last step:  $\langle |\mathbf{R}(s) - \mathbf{R}(s')|^2 \rangle \sim L_p |s - s'|$ . Using the self-avoiding scaling behavior  $\langle |\mathbf{R}(s) - \mathbf{R}(s')|^2 \rangle \sim L_p^{2-2\nu} |s - s'|^{2\nu}$  gives precisely the same result. We thus see that short-distance correlations saturate the rigorous lower bound.

Our long wavelength theory makes a different prediction for the scaling behavior of  $\langle W_I^2 \rangle$ . In section 3, we found the correlation function  $G^C(\mathbf{x}; \mu)$  for a closed polymer loop with a chemical potential  $\mu$  per monomer (3.13). Using this function as a starting point, we determine the scaling behavior of the moments of the writhe. After taking the continuum limit for large  $L$ , we recover the fixed length generating function using an inverse Laplace transform:

$$\overline{\Upsilon}^C(L) = \frac{1}{2\pi i} \oint \overline{G}^C(\mu; g^2) e^{-\mu(L-1)} d\mu \tag{5.5}$$

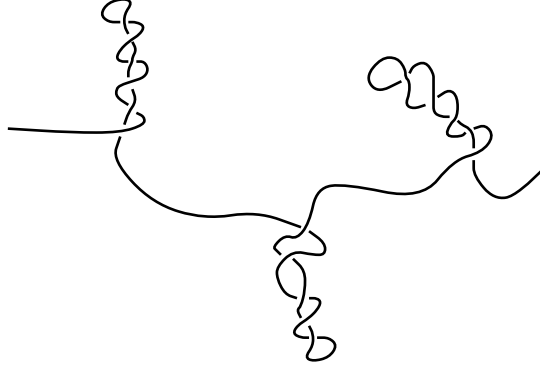


Figure 8: The writhe is dominated by short plectonemic regions separated by distances larger than the persistence length.

where the contour of integration encloses all the poles of the integrand and

$$\overline{G}^C(\mu; g^2) = \lim_{N \rightarrow 0} \frac{1}{N} \langle \vec{\psi}^\dagger(\mathbf{0}) \cdot \vec{\psi}(\mathbf{0}) \rangle \quad (5.6)$$

is the generating function for all closed loops. From this function, the second moment of the writhe for the closed paths is easily obtained:

$$\langle W_I^2 \rangle = \frac{d^2}{d(g^2)^2} \ln \overline{\Upsilon}^C(\mathbf{x}; L) \Big|_{g^2=0}. \quad (5.7)$$

Explicit evaluation of the integral in (5.5) is difficult, but fortunately we are only interested in the way  $\overline{\Upsilon}^C$  scales with  $L$ . We assume a scaling relation for the correlation function,

$$\overline{G}^C(\mu; g^2) = L^{\alpha-1} \overline{G}^C(\mu L; g^2), \quad (5.8)$$

where  $\alpha$  is the specific heat exponent and we have used the fact that  $g^2$  does not rescale. We can now obtain the scaling behavior of  $\overline{\Upsilon}^C$ :

$$\begin{aligned} \overline{\Upsilon}^C(L) &= \frac{1}{2\pi i} \oint L^{\alpha-1} \overline{G}^C(\mu L; g^2) e^{-\mu L} \frac{d(\mu L)}{L} \\ &\sim L^{\alpha-2}. \end{aligned} \quad (5.9)$$

As we saw in the last section, the chemical potential for writhe  $g^2$  does not get renormalized. What is more, this chemical potential does not appear at this order in the scaling exponent of  $\overline{\Upsilon}^C$ . It follows that all of the  $L$  dependence drops out of (5.7) when the derivatives of the logarithm are taken. We conclude that  $\langle W_I^2 \rangle$  does not scale linearly with the length of the chain; at best, the length-dependence enters as some power of a logarithm. Another paradoxical result is obtained when we compute the



average writhe in the presence of a chemical potential:

$$\langle Wr \rangle = -\frac{d}{d(g^2)} \ln \Upsilon^C(L) \sim L^0 \quad (5.10)$$

The length dependence drops out just as it did for the second moment. A chemical potential for writhe does not seem to require the total amount of writhe to grow with the chain length.

These results, though at first surprising, are consistent with existing results. By construction, our field theory only applies to the behavior of the random walk on scales longer than the persistence length. We have seen that the writhe is concentrated on shorter length scales, and so we would not expect to see it in this field theoretic treatment. A picture emerges of short plectonemic regions separated from each other by at least the polymer persistence length (see fig. 8). These plectonemic regions each contribute to the writhe of the polymer, but these contributions appear only as matching conditions in our long wavelength theory. We would therefore expect that in the presence of a chemical potential for writhe, the average writhe of the chain *will* scale with the chain length:

$$\langle Wr \rangle \approx \frac{L}{L_p} \langle Wr \rangle_{\text{pl}}, \quad (5.11)$$

where  $\langle Wr \rangle_{\text{pl}}$  is the average writhe per plectonemic segment. Likewise, the second moment is dominated by the small plectonemic regions:

$$\langle Wr^2 \rangle \approx \frac{L}{L_p} \langle Wr^2 \rangle_{\text{pl}}. \quad (5.12)$$

It might seem strange to talk about the writhe of a short segment of the polymer when writhe is a global property of the entire chain. But as can be seen from the  $|\mathbf{R}(s) - \mathbf{R}(s')|^{-3}$  factor in (2.3), the writhe is dominated by the correlations between regions that are close together in space.

## 6 Conclusion

In this paper we have investigated the topology of self-avoiding random walks. Our goal was to understand how the linking number constraint changes the conformational statistics of closed polymers. After integrating out the twist degree of freedom, this problem was shown to be equivalent to that of studying the statistics of a polymer with a chemical potential for writhe. By mapping this modified problem onto the  $N \rightarrow 0$  limit of an  $O(N)$  complex scalar field theory with a Chern-Simons gauge field, we were able to find that the presence of a small chemical potential for writhe does not change the

behavior of our polymer in the scaling limit: that is, the renormalization group equations for the ungauged scalar field model that describes the usual self-avoiding walk do not get modified by the introduction of the Chern-Simons term. We also saw that a sufficiently large chemical potential,  $g^2 \gtrsim (\pi/2)$ , collapses the polymer.

We carried out our perturbation expansion to one loop. The anomalous wavefunction renormalization of  $\psi$  at the Wilson-Fisher fixed point kept all of the possible corrections to scaling finite; this result should be compared to that of naïve power counting where logarithmic divergences occur. In view of this, it is reasonable to believe that the renormalization group equations do not change to all orders in the loop expansion. It would be interesting to carry out a careful analysis of the power counting at the Wilson-Fisher fixed point. It may also be possible to adopt the wealth of knowledge on anyons [22] to study the critical behavior of our model as well as the use of supersymmetry [23] to study self-avoiding walks.

Additionally, we investigated the scaling behavior of the writhe itself. We found that the long wavelength contribution to the writhe does not scale with its length. The writhe escapes the notice of the scaling theory by hiding at small scales. We find our results to be consistent with a picture whereby the writhe is confined mainly to short plectonemic segments separated by at least the bend persistence length.

Our overall results indicate that the effects of topology do not change the general scaling properties of polymers: constrained random walks belong to the same universality class as unconstrained ones. The effects of topology seem to enter only on small scales through the chemical and physical details of the chain.

Recently [25] the winding number statistics of directed polymers have been analyzed by adding an auxiliary  $2 + 1$  dimensional gauge field. We note that the Chern-Simons formalism presented here can be used to study the linking number statistics of an ensemble of closed, *isotropic*, polymer loops, as can be found, for instance, in the kinetoplast DNA of trypanosomes [24]. The rheological properties of these so-called “olympic gels” are intimately connected to their topology. Thus, via bulk experiments, the linking number statistics could be explored.

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